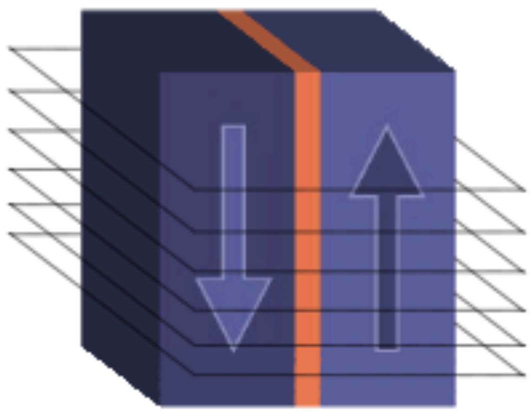
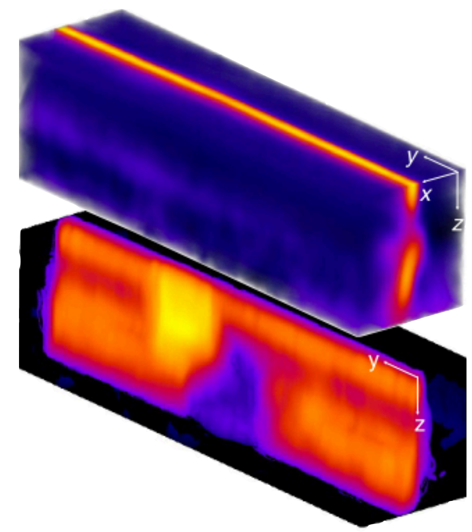
Domain walls in ferroelectric materials:

outstanding functional nano-entities with unique physical properties





DQMP Seminar - Salia Cherifi-Hertel

Cherifi-Hertel et al.,

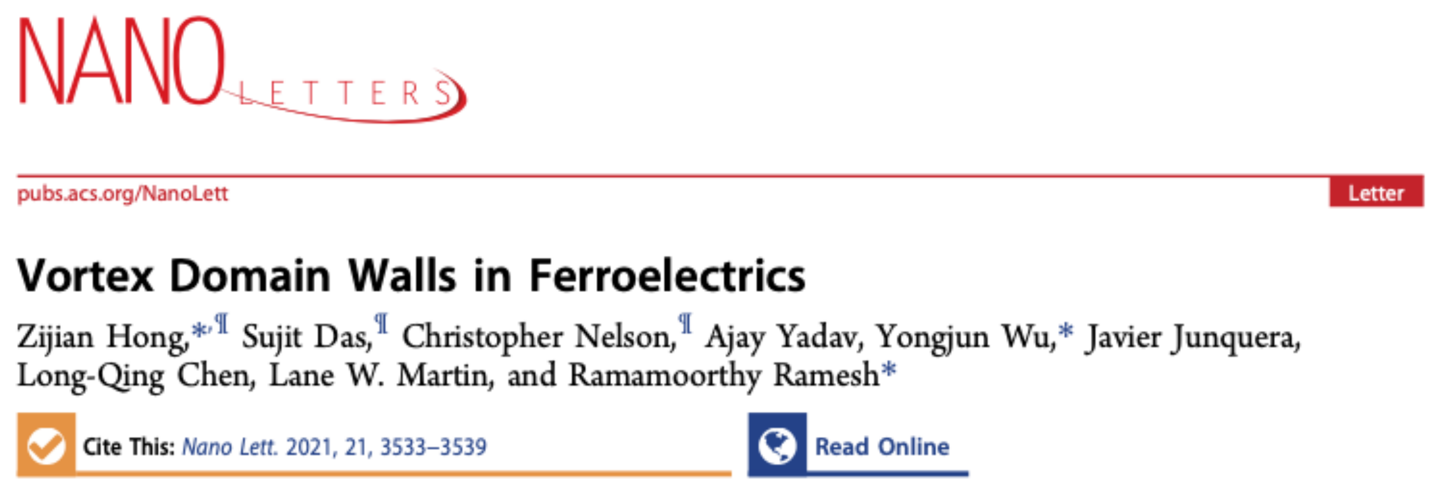
Nature Comm. 8:15768 (2017)

Outline:

- Basic concepts:
  - Ferroelectricity
  - Domains
  - Domain walls

- Domain wall properties

- Vortex domain walls in ferroelectrics


NANO LETTERS

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Vortex Domain Walls in Ferroelectrics

Zijian Hong,*,¶ Sujit Das,¶ Christopher Nelson,¶ Ajay Yadav, Yongjun Wu,* Javier Junquera, Long-Qing Chen, Lane W. Martin, and Ramamoorthy Ramesh*

Cite This: *Nano Lett.* 2021, 21, 3533−3539 Read Online

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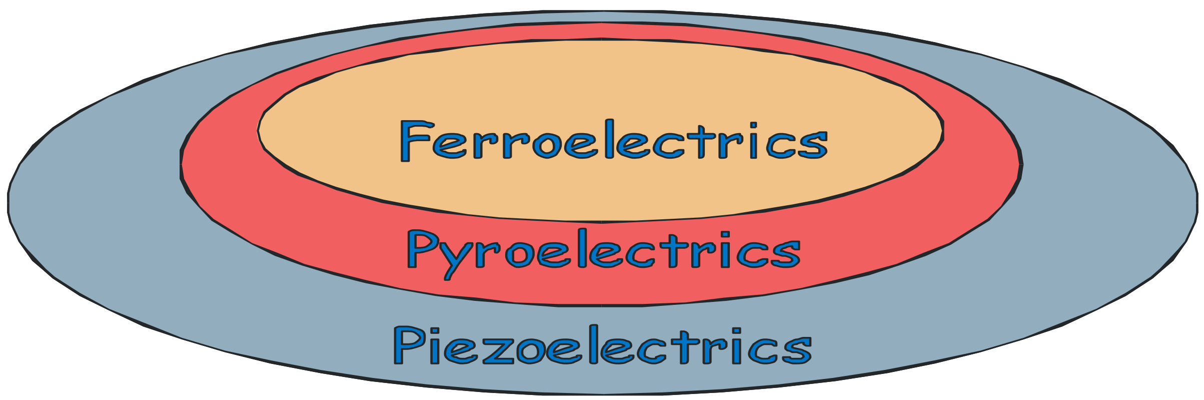
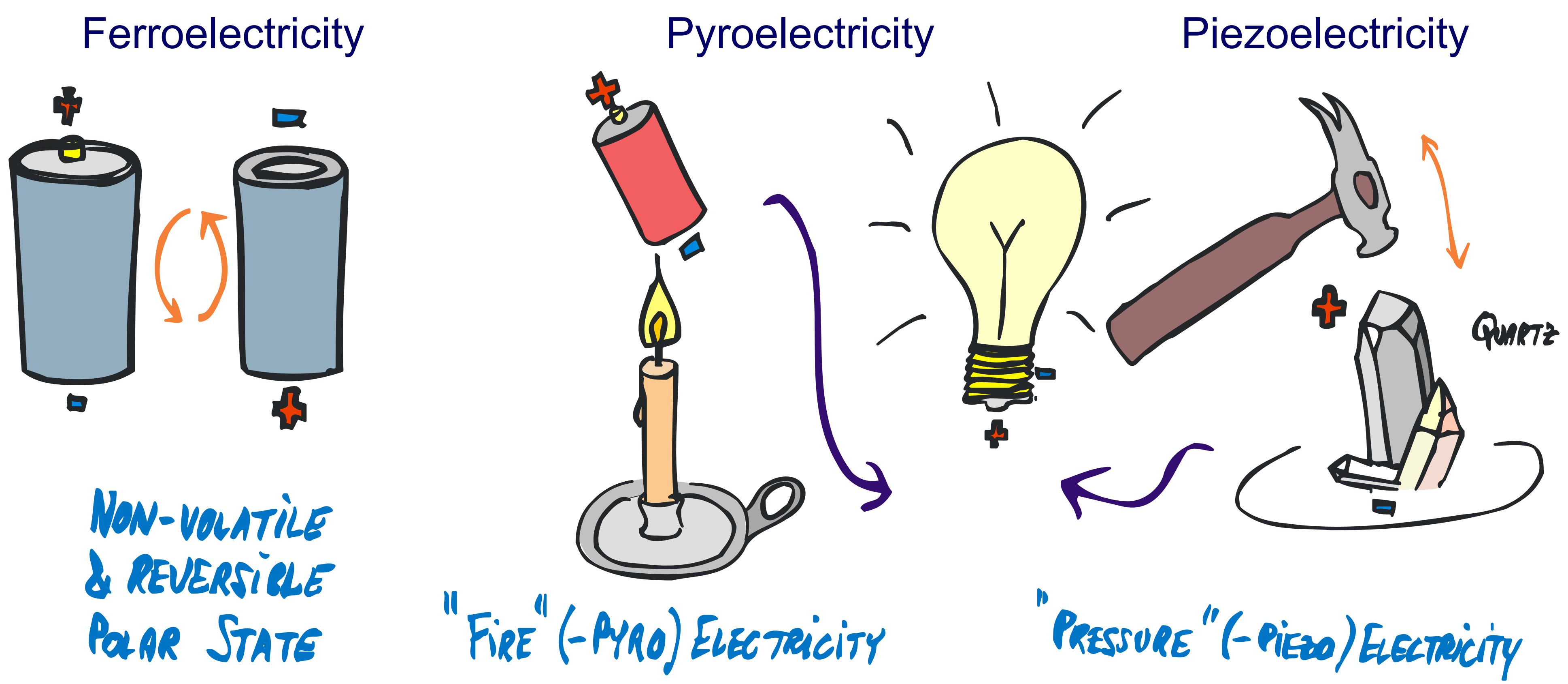
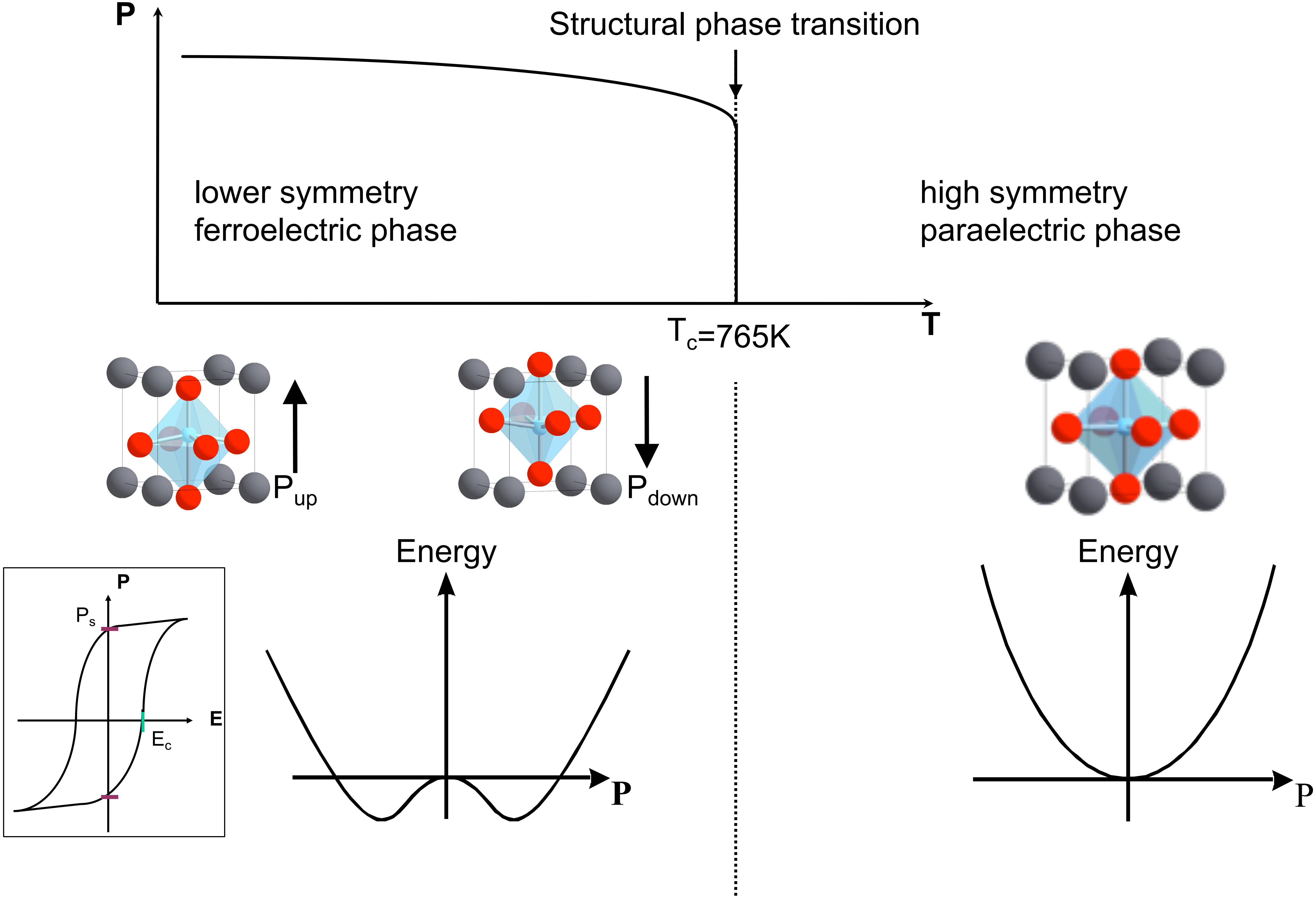
Ferroelectricity





Kuffer, MaNEP Newsletter Nr.6 (spring 2004)

Bulk $PbTiO_3$



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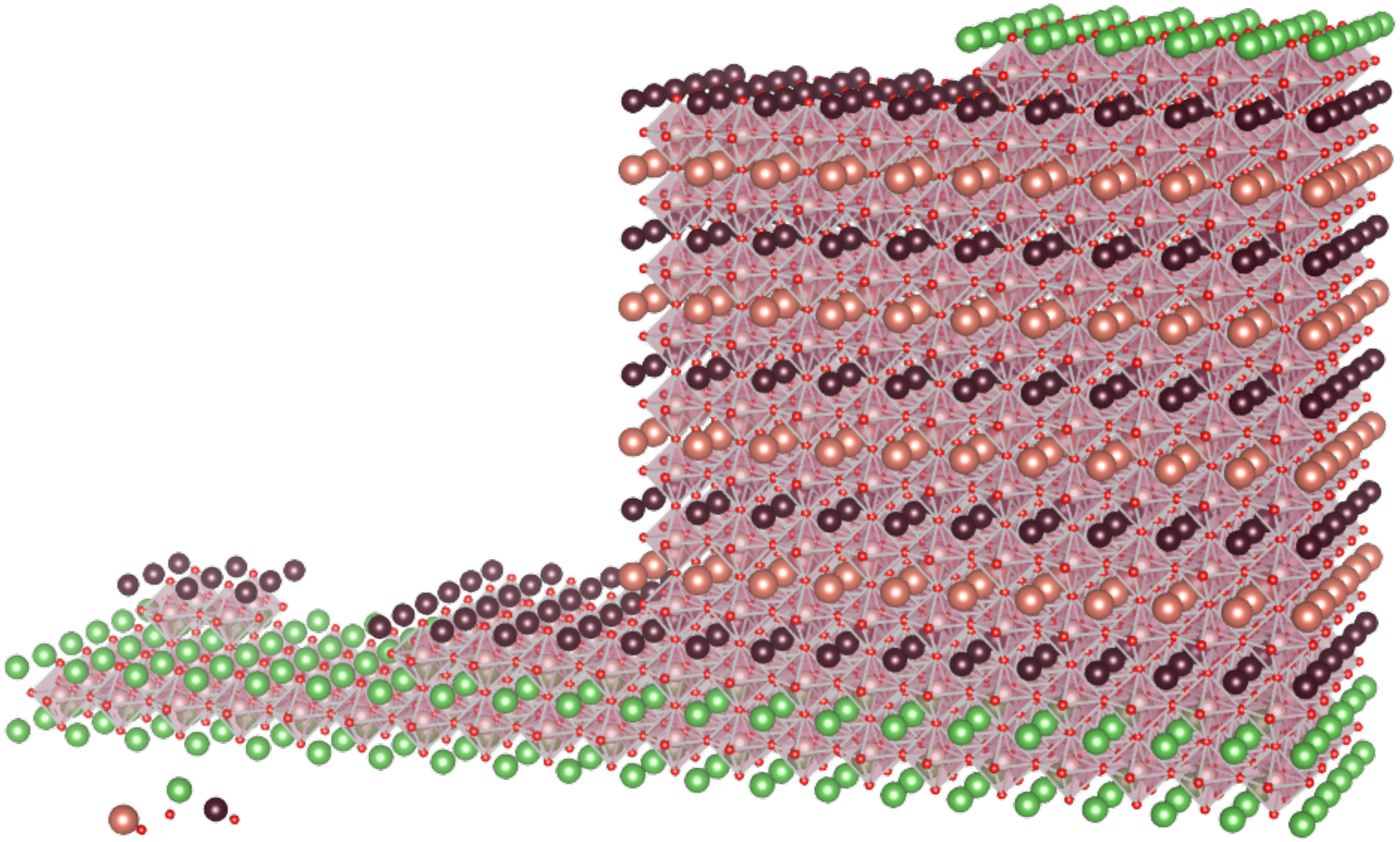
Epitaxial thin films



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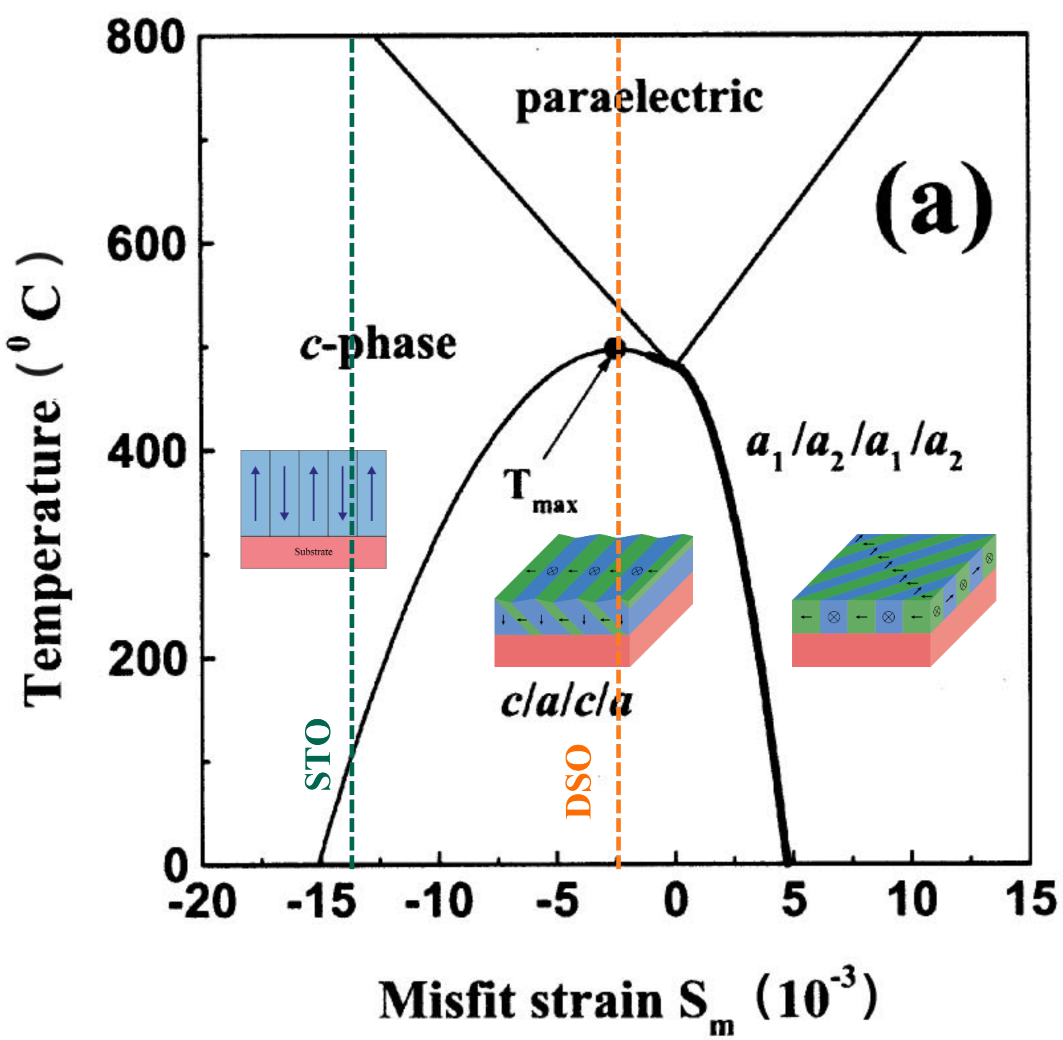
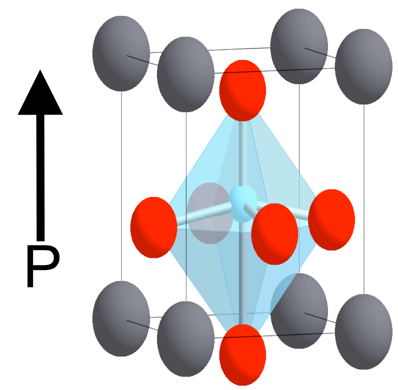
Effect of strain

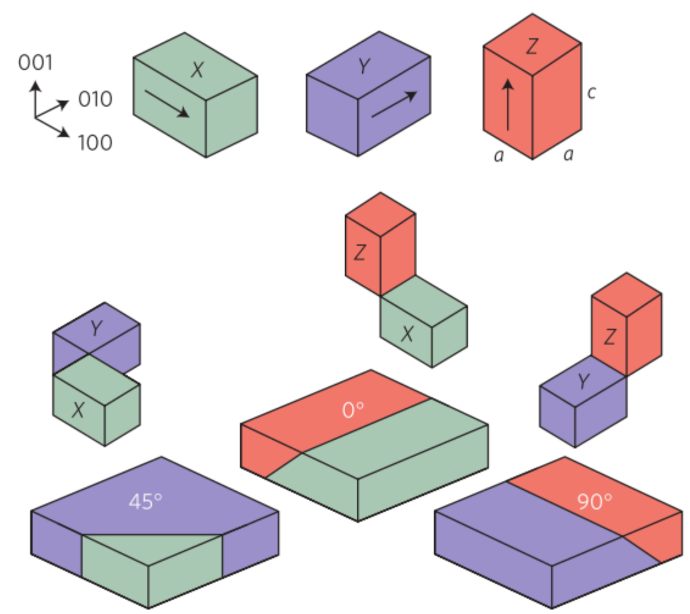
Bulk lattice parameters @RT:

- **$PbTiO_3$**: a=b=3.904Å, c=4.158Å
- **$SrTiO_3$**: a=b=c=3.905Å
- **$SrRuO_3$**: a=b=3.924Å, c=3.925Å
- **$DyScO_3$**: a=c=3.946Å, b=3.952Å

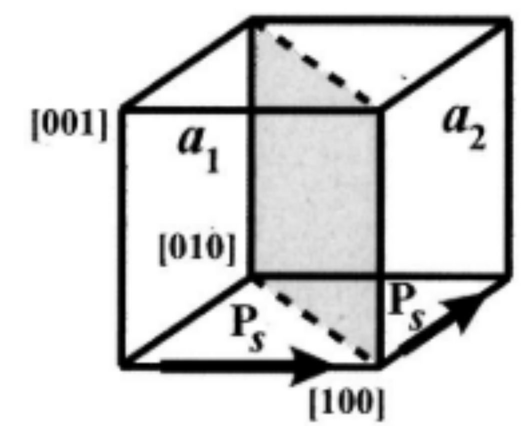


Koukhar, Pertsev and Waser, Phys. Rev. B 64 214103 (2001)

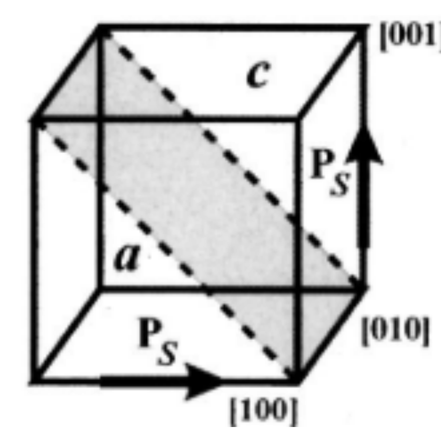




Honig et al. Nat. Mater. 12, 1112 (2013)



$a_1/a_2/a_1/a_2$



c/a/c/a

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- $SrTiO_3$: a=b=c=3.905Å
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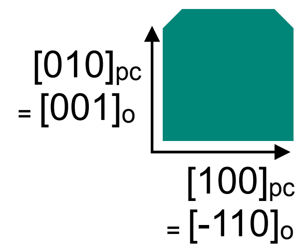
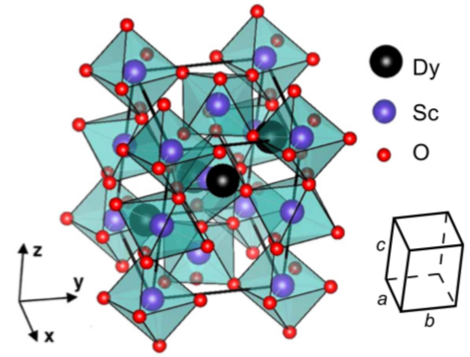
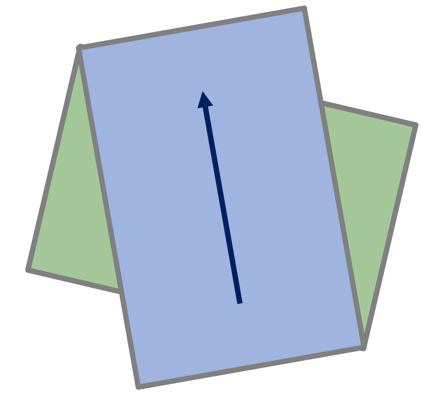
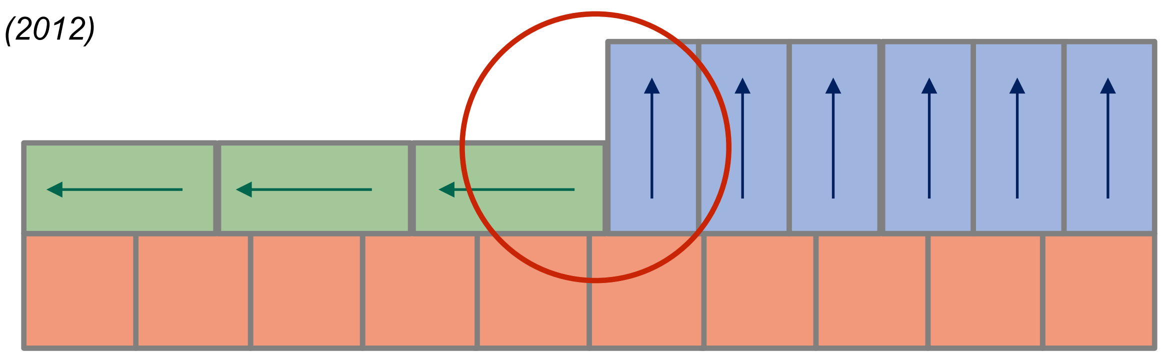
Orthorhombic substrate $DyScO_3$

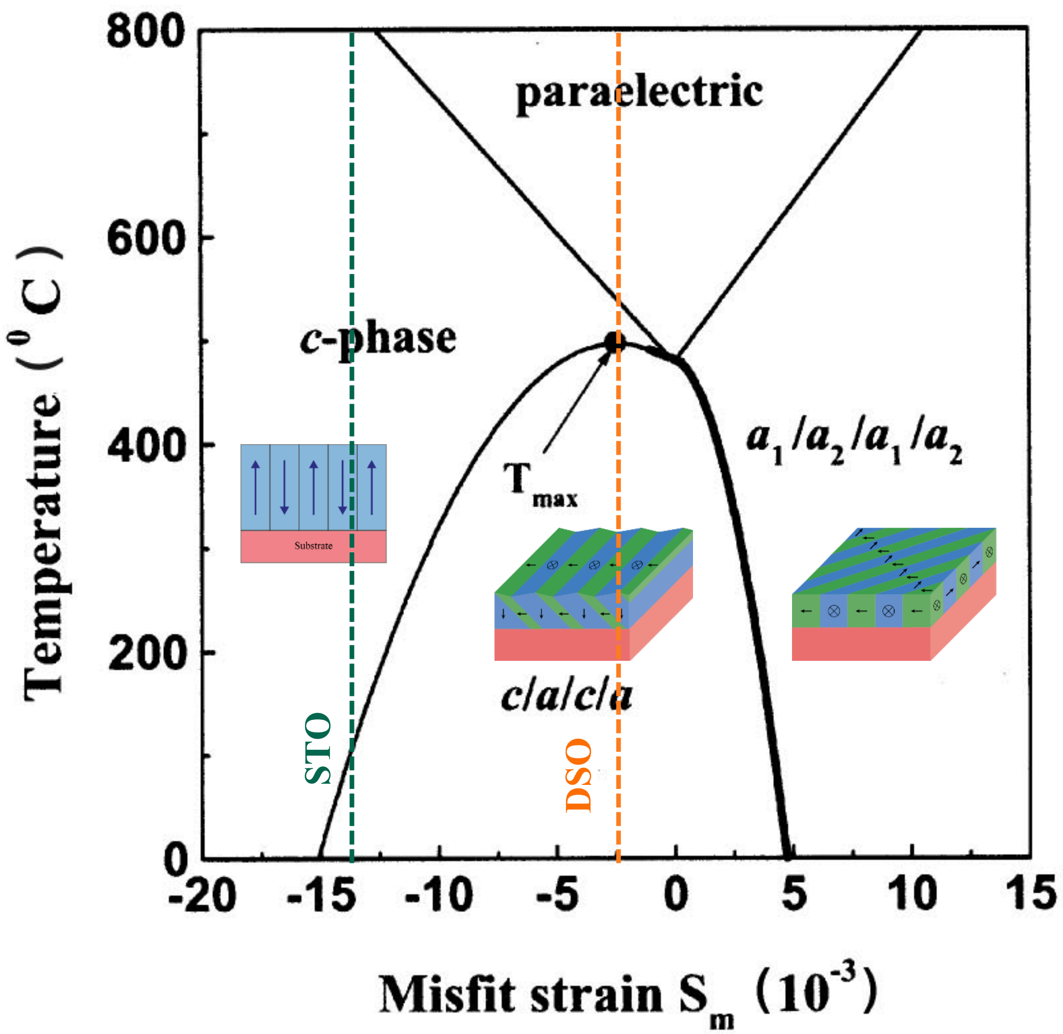




Janovskà, JPCM 24 385404 (2012)

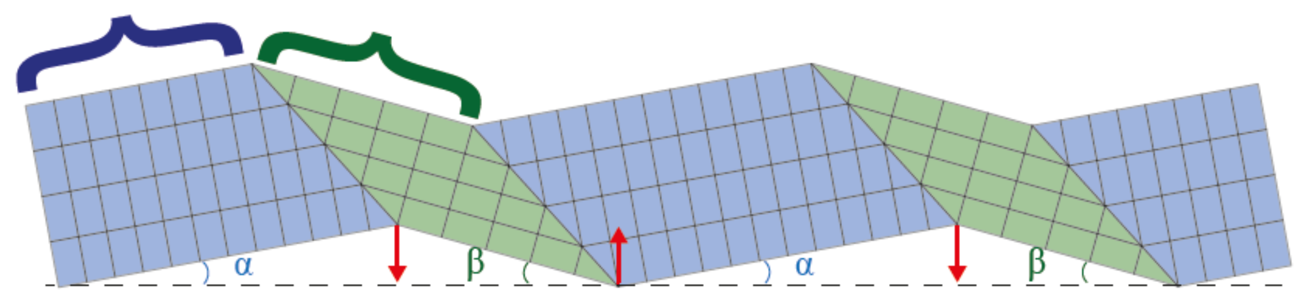


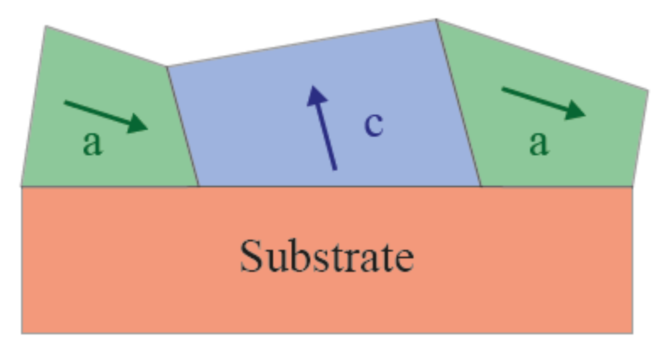




Koukhar, Pertsev and Waser, Phys. Rev. B 64 214103 (2001)

90° ferroelastic domain walls in $PbTiO_3$ thin films





see Catalan et al, Nat. Mater. 10, 963 (2011)

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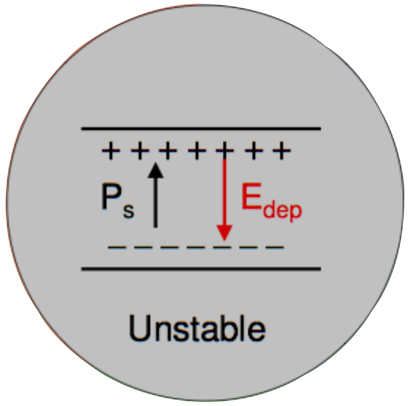
Depolarization field

*Batra and B. Silverman, **Solid State Commun.1972***

*Dawber, Jung and Scott, **APL 2003***

*Dawber, Chandra, Littlewood and Scott, **J. Phys. Condens. Matter 2003***

*Stengel and Spaldin, **Nature 2006***



$E_{dep}=P/\varepsilon_r$

Typical ferroelectric:
$P=10\mu C/cm^2$
$\varepsilon_r=100\text{-}1000$
$\rightarrow E_{dep}=10\text{-}100kV/cm$

Ferroelectricity in ultrathin-film capacitors
Lichtensteiger, Zubko, Stengel, Aguado-Puente, Triscone, Ghosez and Junquera, chapter 12 in
Oxide Ultrathin Films: Science and Technology, Wiley 2012
arXiv:1208.5309v1

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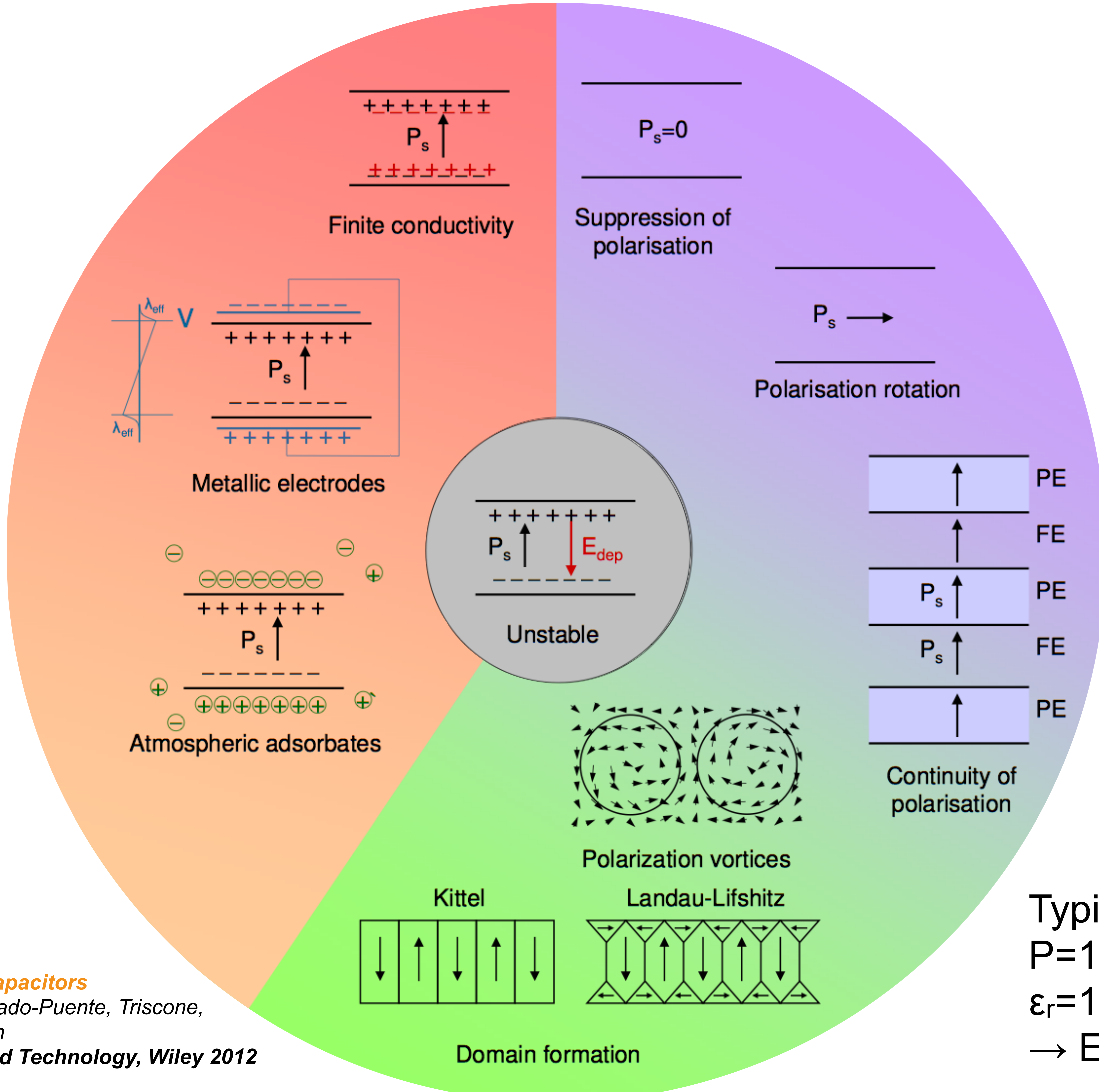

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Landau-Lifschitz-Kittel law

*L. Landau and L. Lifschitz, **Phys. Z. Sowjetunion** 1935*
*C. Kittel, **Phys. Rev.** 1946*

*Catalan, Seidel, Ramesh, Scott, **Reviews of Modern Physics**, 2012*

*Catalan, Scott, Schilling, Gregg, **J. Phys.: Condens. Matter** 2007*

*Scott, **J. Phys. Condens. Matter** 2006*

*Meyer and Vanderbilt, **PRB** 2002*

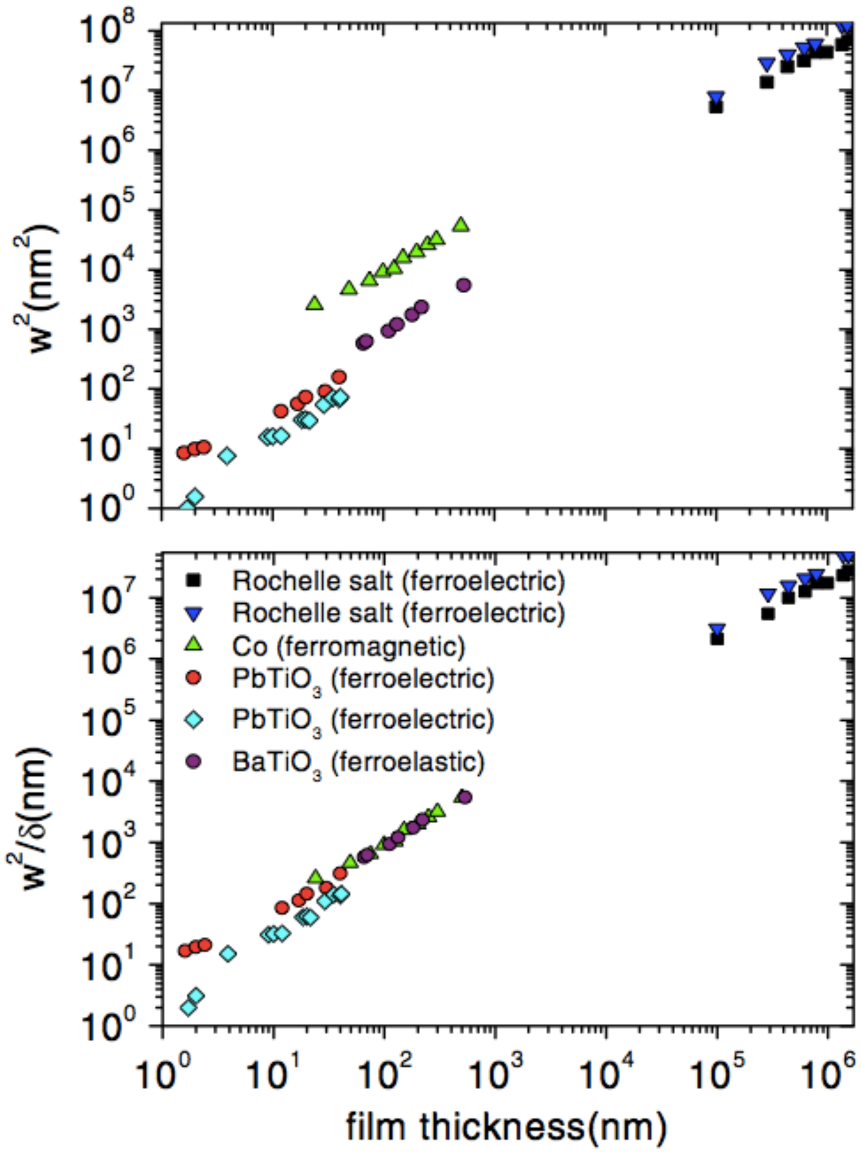
*Streiffer et al. **PRL** 2002*

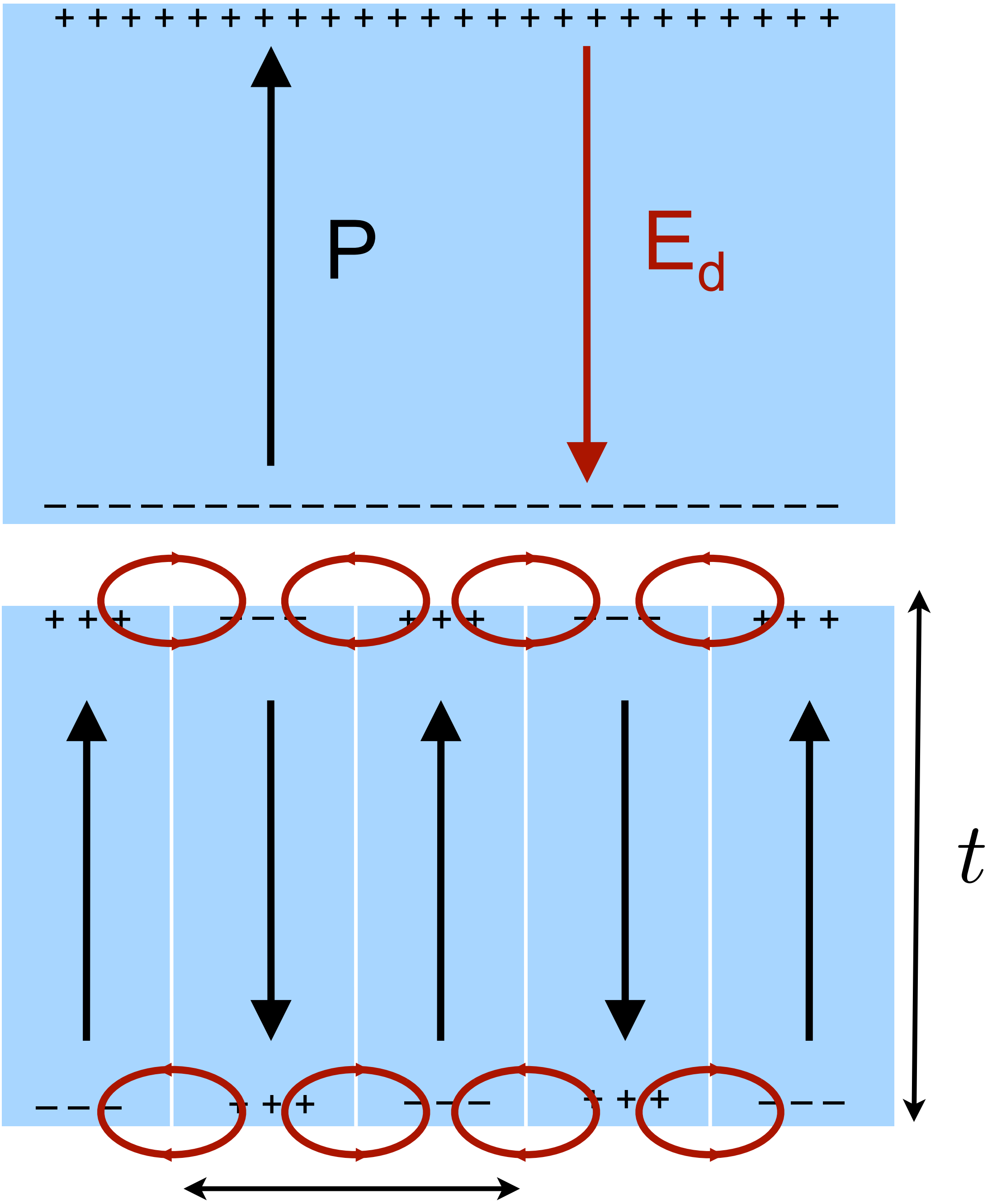
*Hubert and Schäfer, **Springer**, Berlin 1998*

*Hehn, Padovani, Ounadjela, Bucher, **PRB** 1996*

*Pertsev and Zembilgotov, **JAP** 1995*

*J. Mitsui and J. Furuichi, **Phys. Rev.** 1953*





$$F_P \sim P_s^2 \omega$$

$$F_\omega = \sigma_\omega \frac{t}{\omega}$$

$$\omega \sim \sqrt{t}$$

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Domain walls in $PbTiO_3$ thin films

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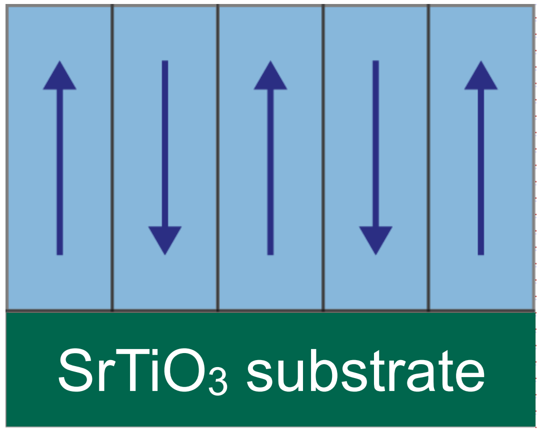
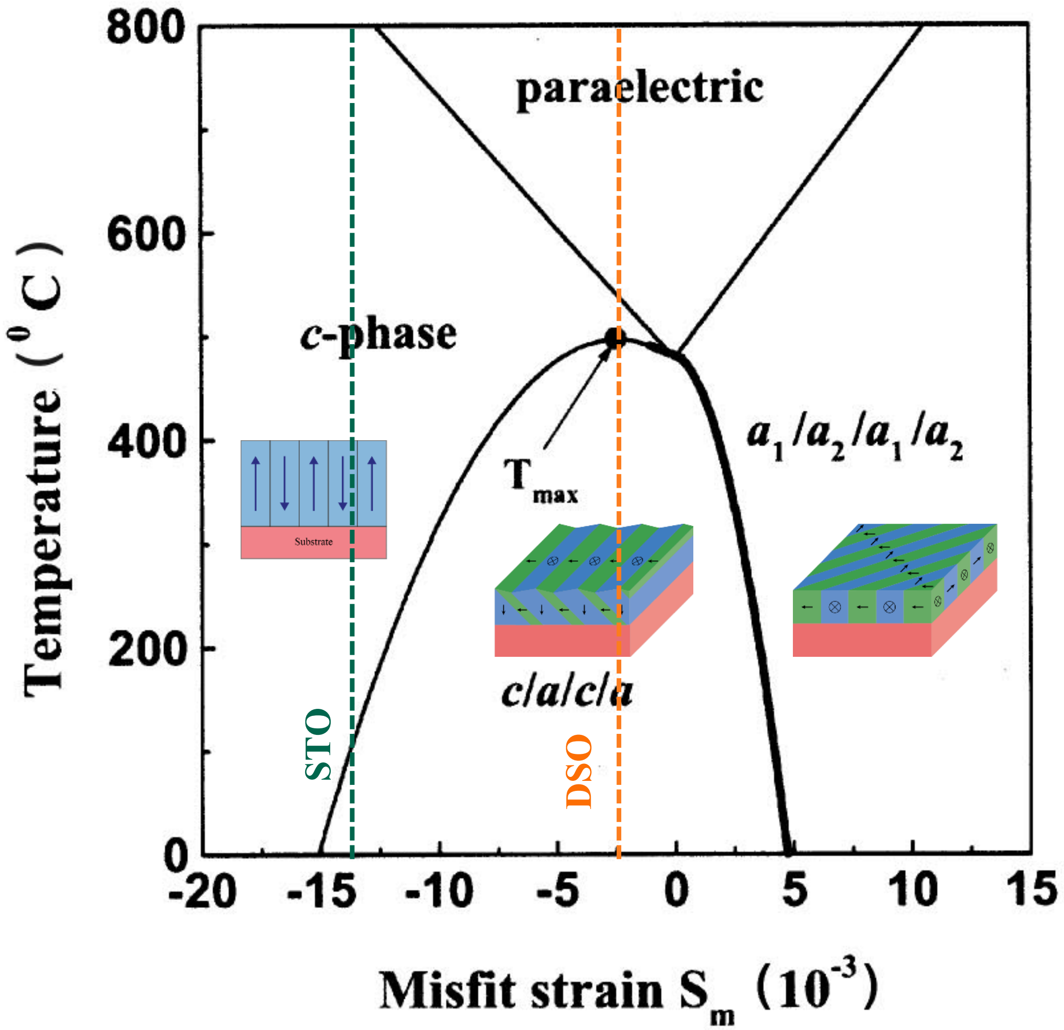
- **$SrRuO_3$**: a=b=3.924Å, c=3.925Å
- **$DyScO_3$**: a=c=3.946Å, b=3.952Å

Electrostatic boundary conditions

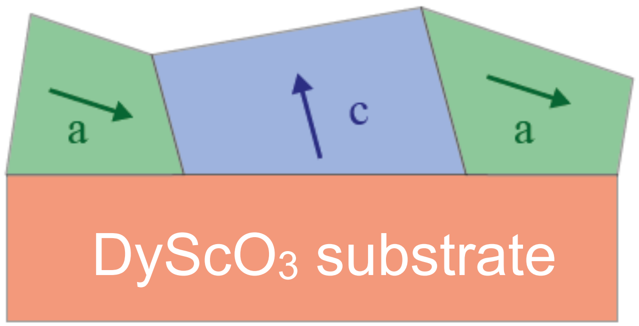
Ferroelectric 180° domain walls





Mechanical boundary conditions

Ferroelastic 90° domain walls



Koukhar, Pertsev and Waser, Phys. Rev. B 64 214103 (2001)

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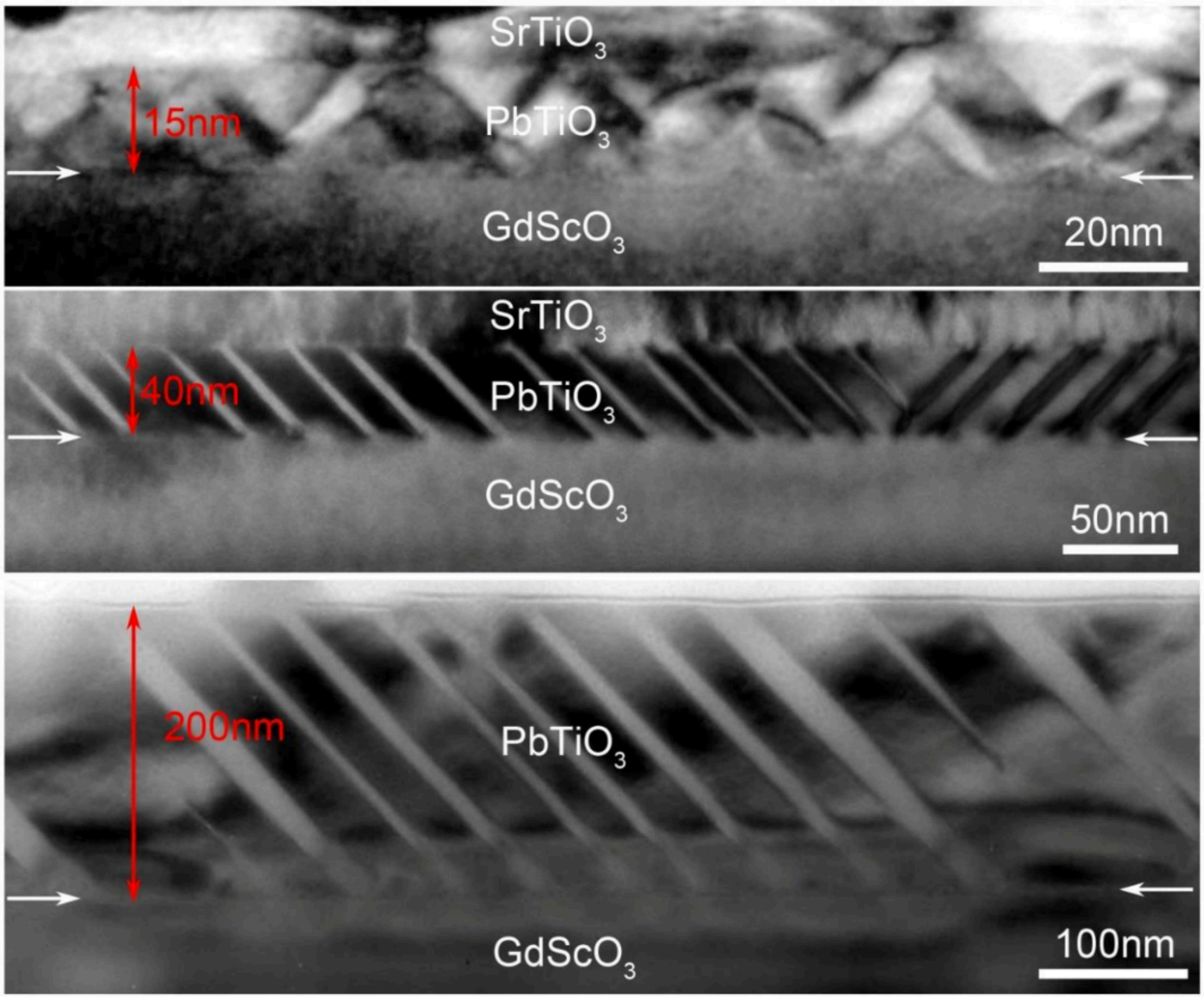
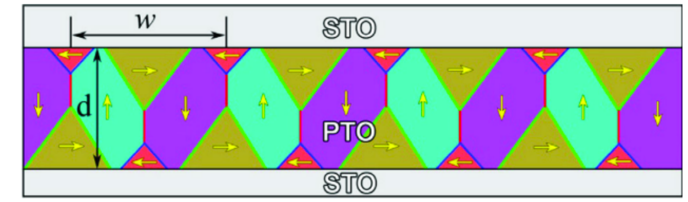
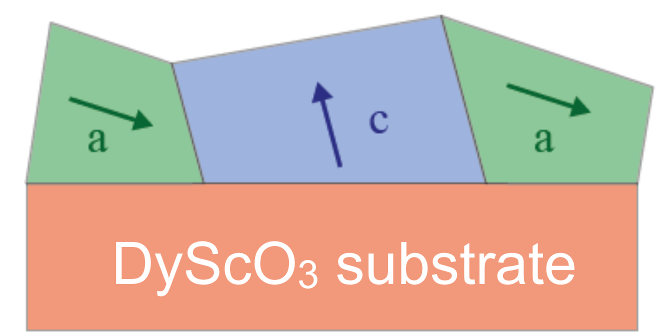


Tang et al, Science 348, 547 (2015)

Flux-closure domain pattern



a/c - Ferroelastic 90° domain walls



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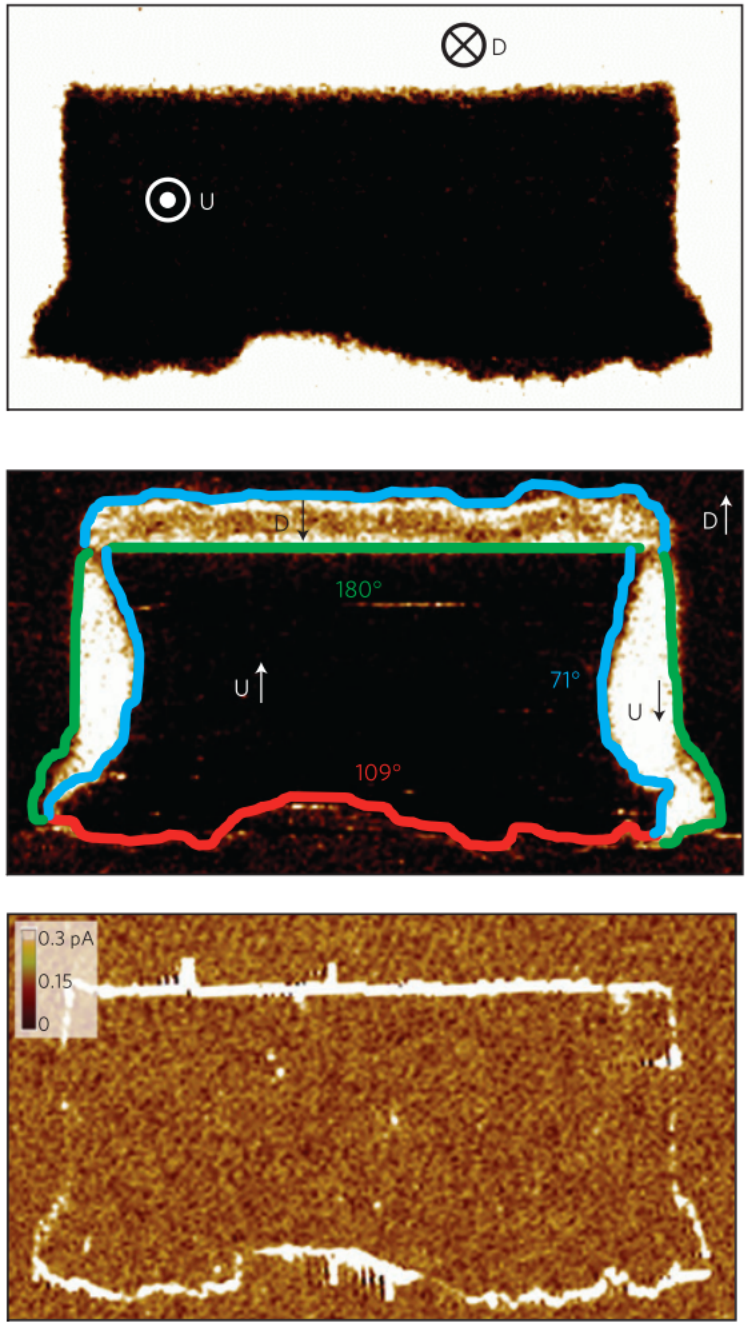
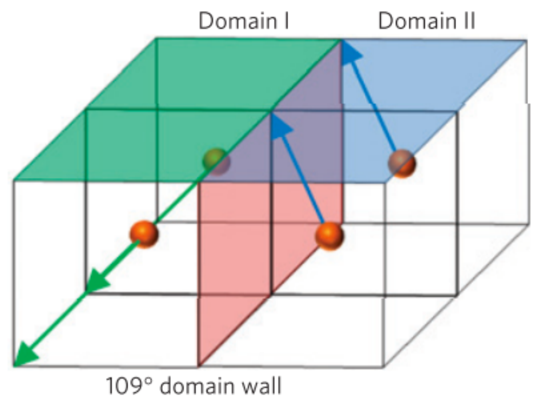
Conduction at domain walls





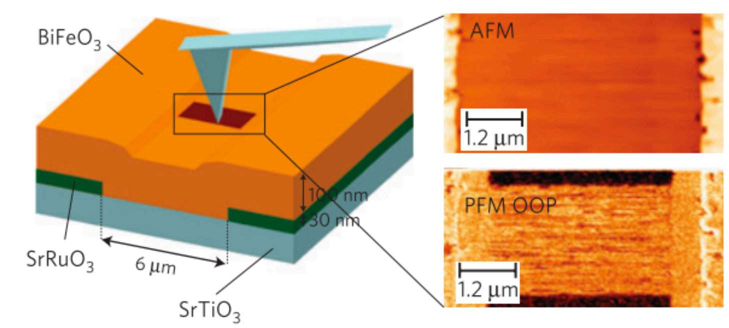
(110) $BiFeO_3$

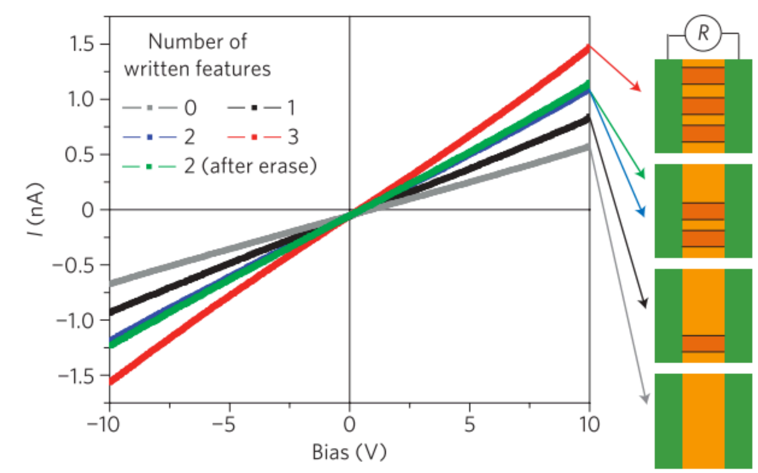
Conduction at 109° and 180° domain walls
No conduction at 71° domain walls

Table 1 | Electronic structure at ferroelectric domain walls.

Domain wall type (°)	Electrostatic potential step (eV)	Change in bandgap (eV)
71	0.02	0.05
109	0.15	0.10
180	0.18	0.20

Calculated values of the potential step and reduction in bandgap at all three domain-wall types.





Proof of concept for device application

Conduction at domain walls in oxide multiferroics

Seidel et al, Nature Materials 8:229(2009)

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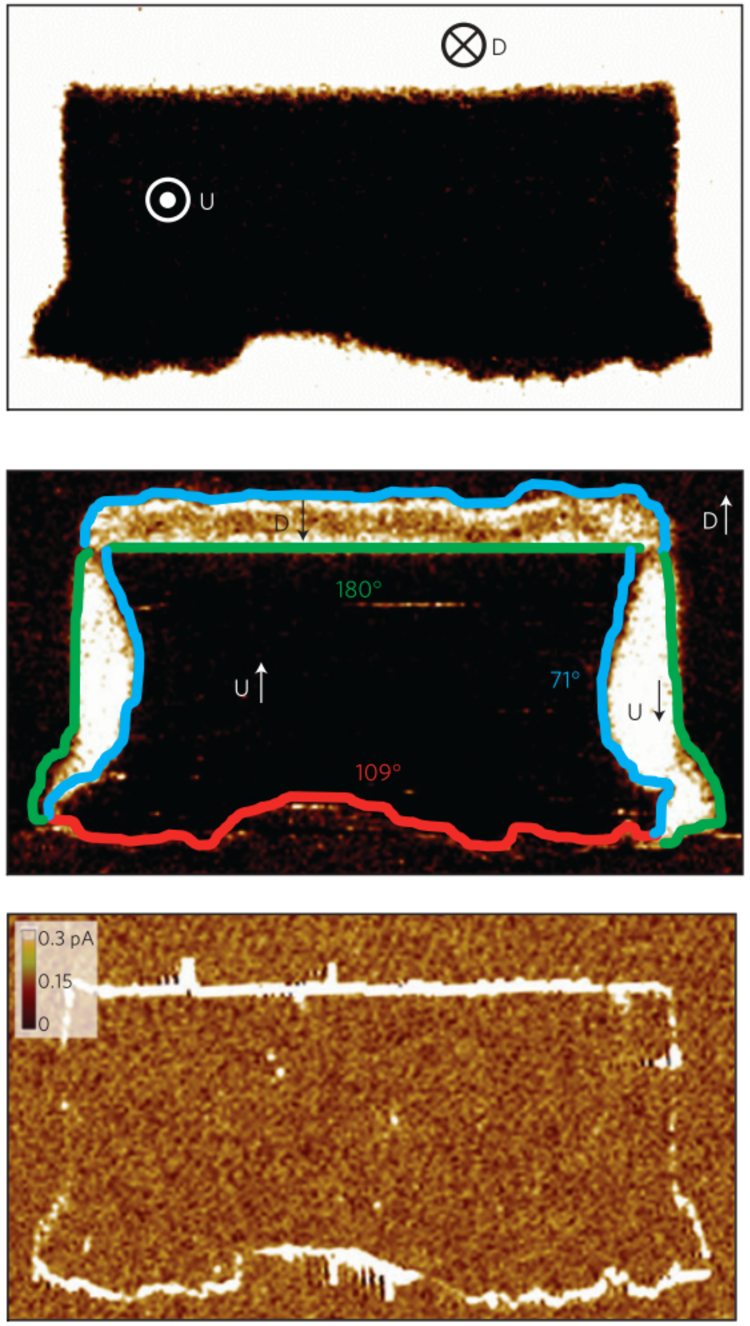
Conduction at domain walls



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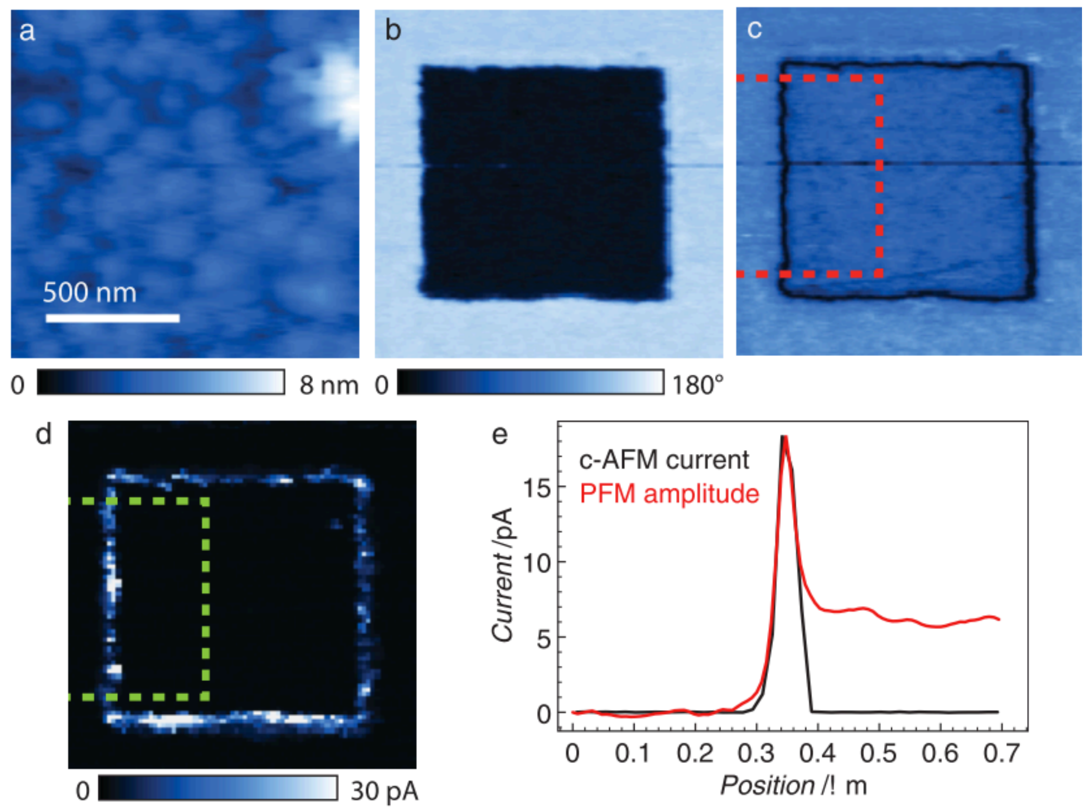

Conduction at 180° domain walls

$PbZr_{0.2}Ti_{0.8}O_3$

Conduction at domain walls in oxide multiferroics

Seidel et al, Nature Materials 8:229(2009)

Conduction at domain walls in insulating $Pb(Zr_{0.2}Ti_{0.8})O_3$ thin films

Guyonnet, Gaponenko, Gariglio, Paruch, Advanced Materials 23:5377(2011)

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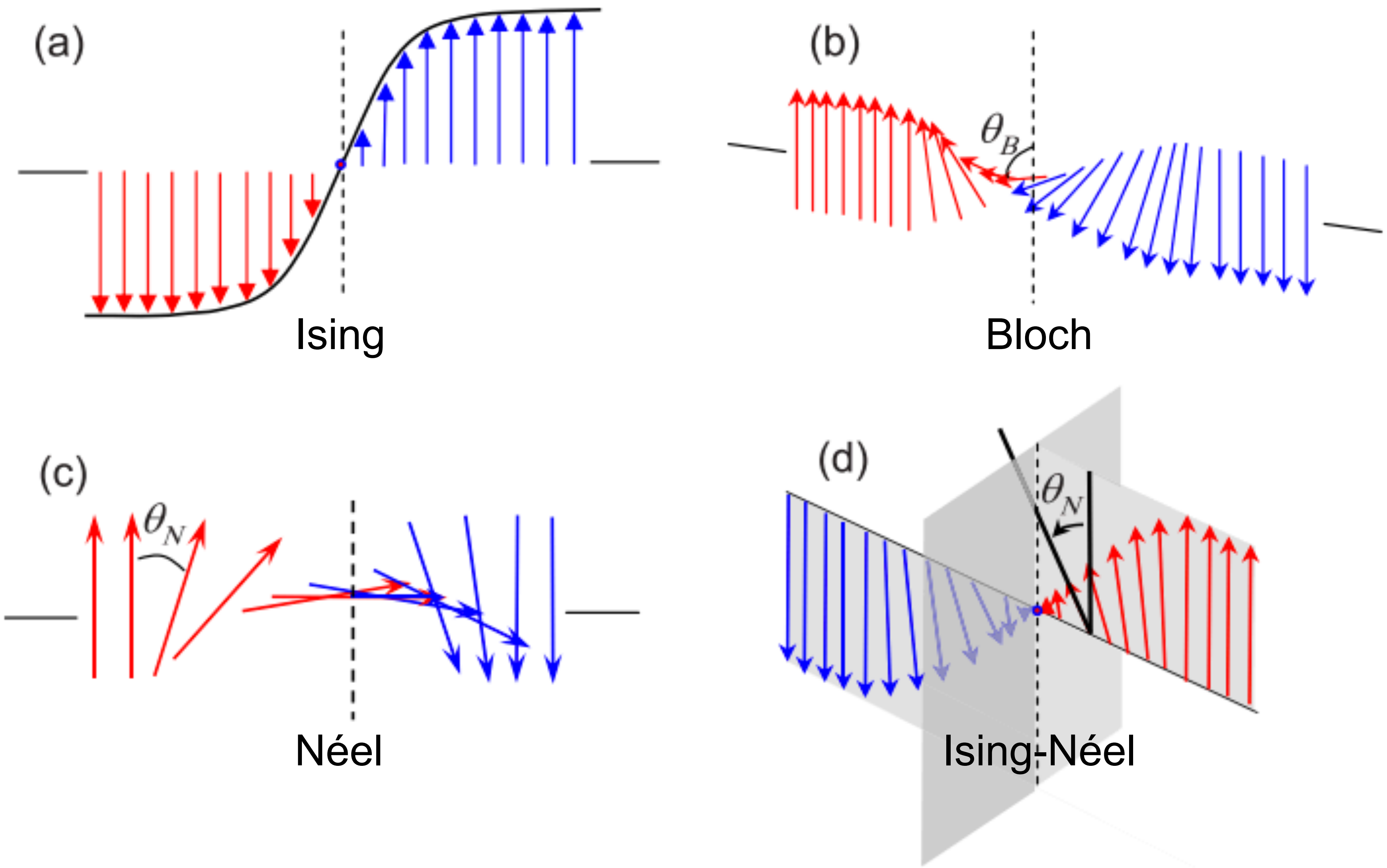
Nature of 180° ferroelectric domain walls

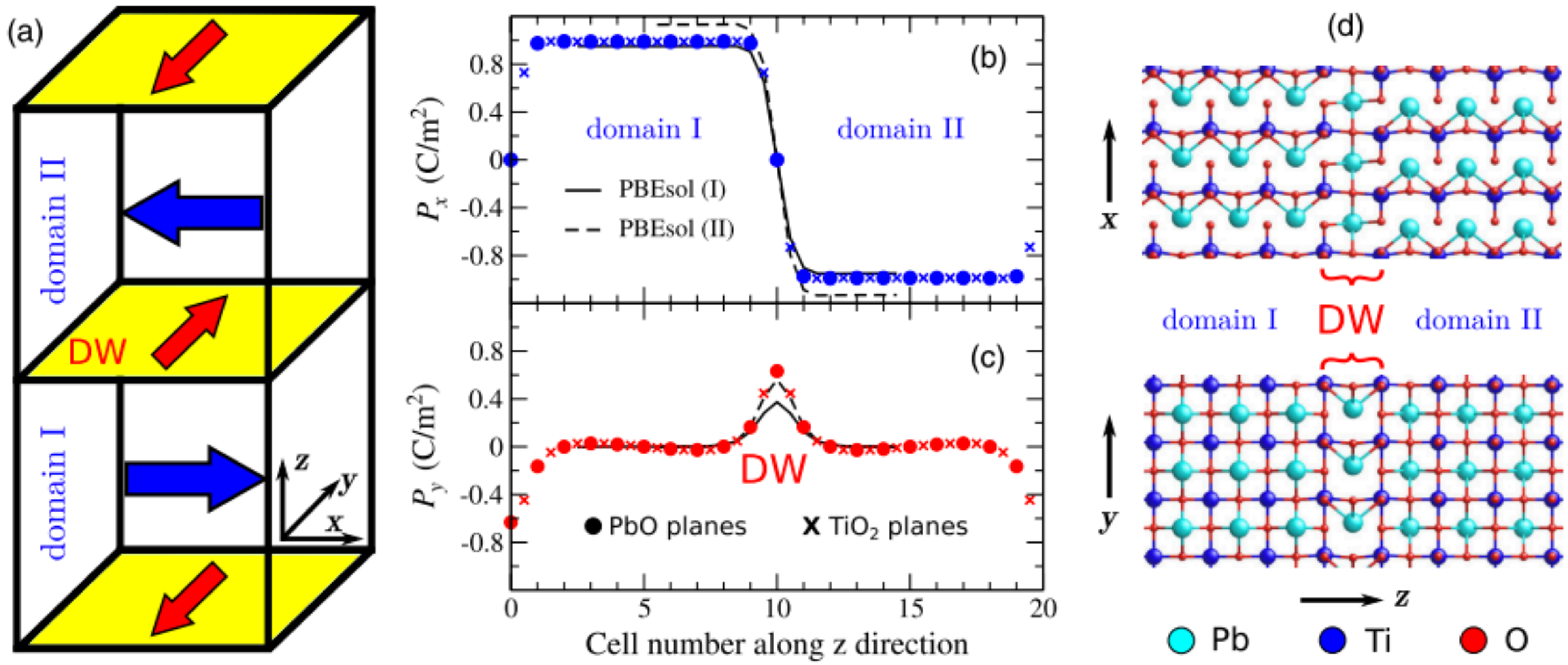


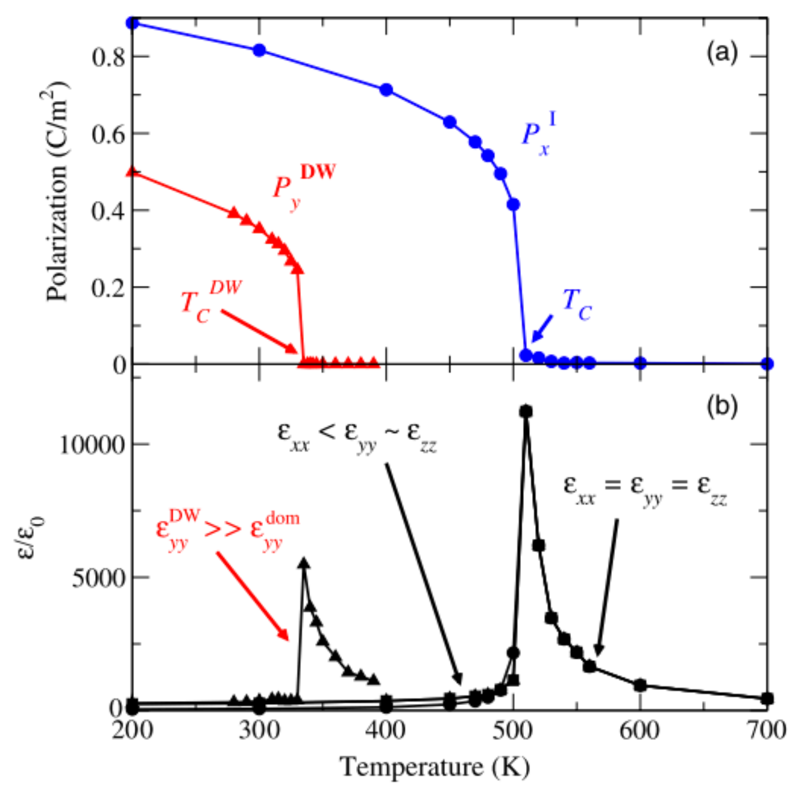
Mixed Bloch-Néel-Ising character of 180° ferroelectric domain walls

Lee, Behera, Wu, Xu, Li, Sinnott, Phillpot, Chen, Gopalan,

Phys. Rev. B 80, 060102 (2009)

Nature of 180° ferroelectric domain walls





Ferroelectric Transitions at Ferroelectric Domain Walls Found from First Principles
Wojdeł and Íñiguez, PRL 112, 247603 (2014)

From Ising (P=0) to Bloch (P≠0, switchable) at low T.

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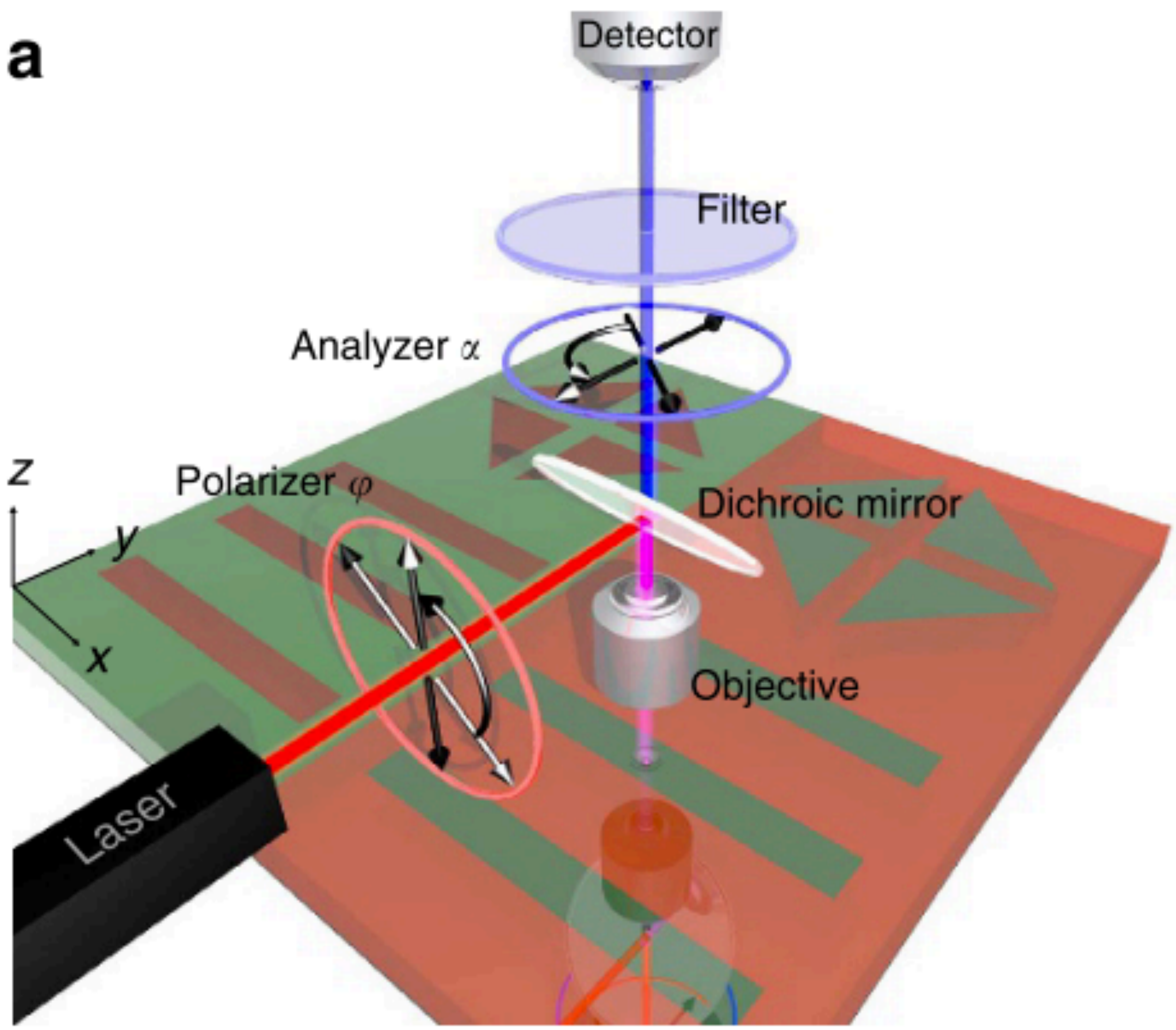
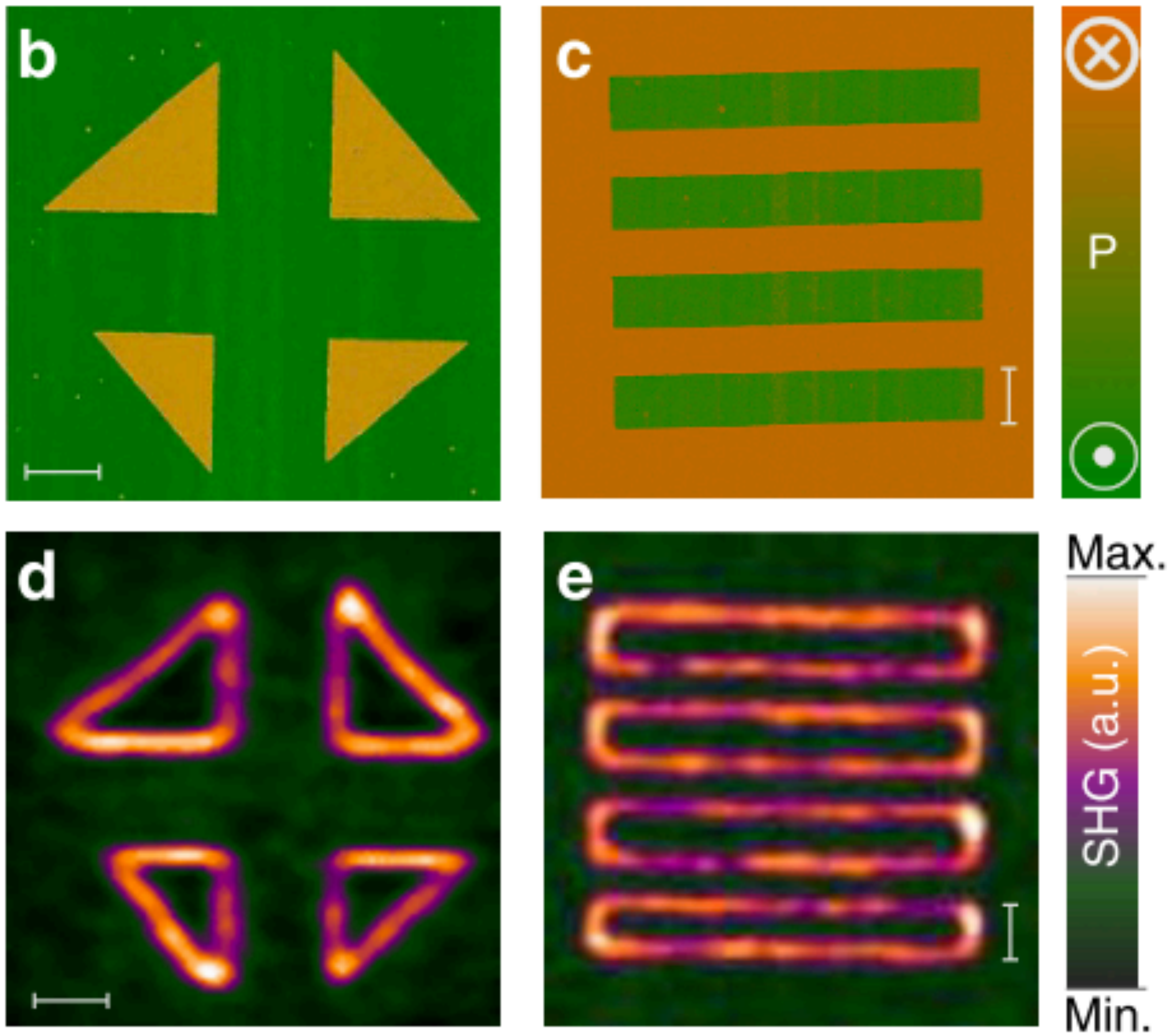
Nature of 180° ferroelectric domain walls





50 nm-thick $PbZr_{0.2}Ti_{0.8}O_3$

Non-Ising and chiral ferroelectric domain walls revealed by nonlinear optical microscopy

Cherifi-Hertel, Bulou, Hertel, Taupier, Dorkenoo, Adreas, Guyonnet, Gaponenko, Gallo, Paruch, Nature Comm. 8:15768 (2017)

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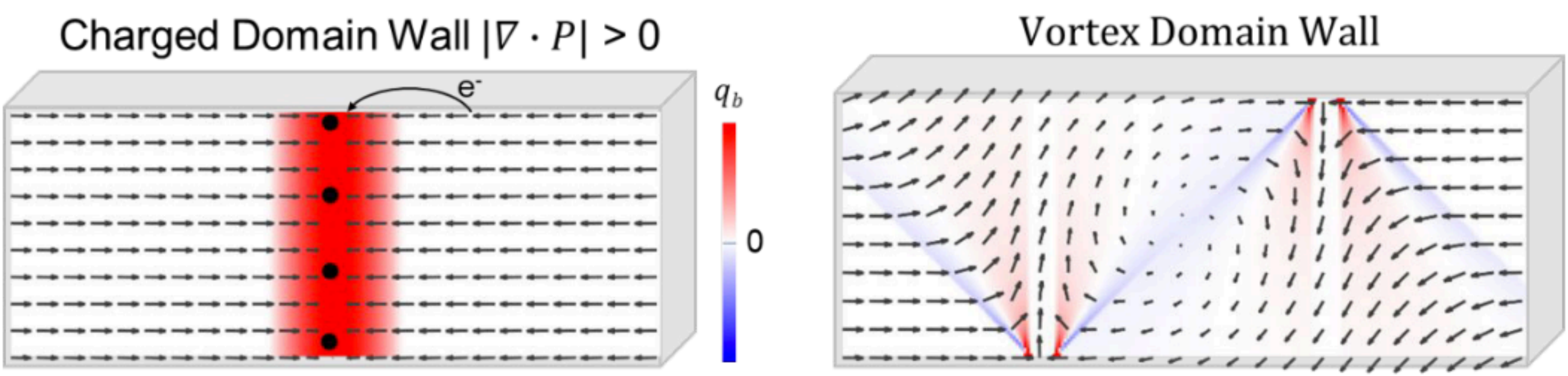
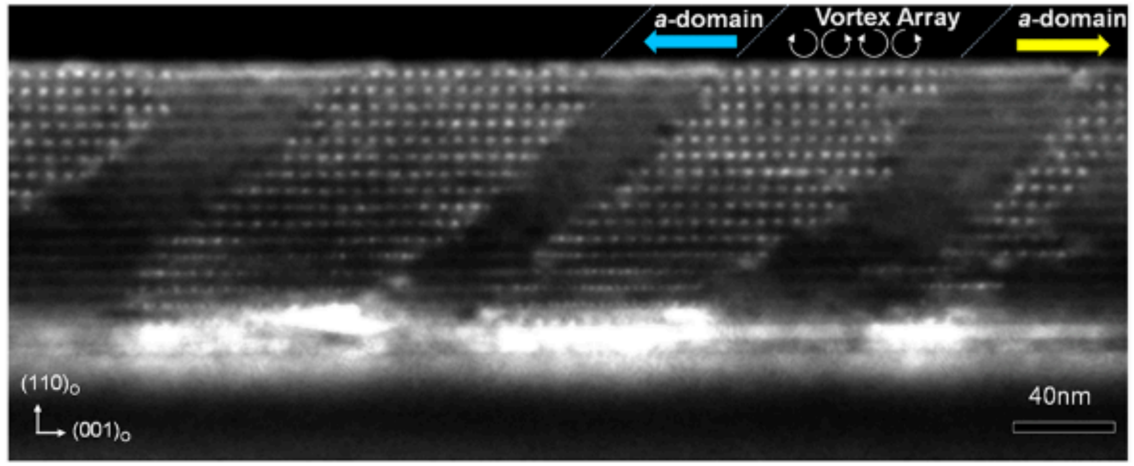


Vortex Domain Walls in Ferroelectrics
Hong, Das, Nelson, Yadav, Wu, Junquera, Chen, Martin, Ramesh, Nano Letters 21 3533 (2021)

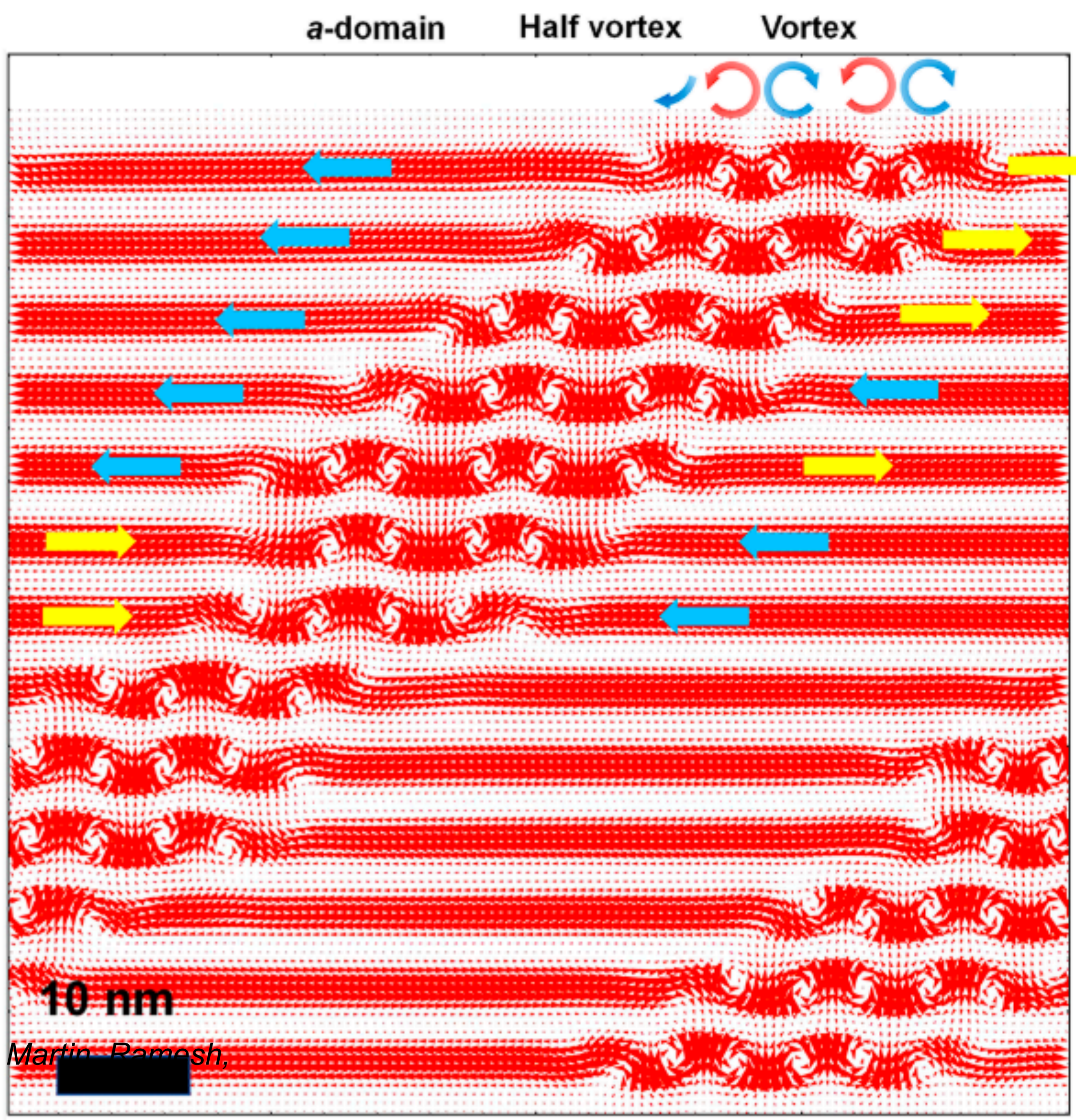
Vortex Domain Walls in Ferroelectrics



$(PbTiO_3)_6/(SrTiO_3)_6$ superlattice

$SrRuO_3$ electrode

$DyScO_3$ substrate



"head-to-tail" (neutral)
"tail-to-tail" (charged)
"head-to-head" (charged)

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Nano Letters 21 3533 (2021)

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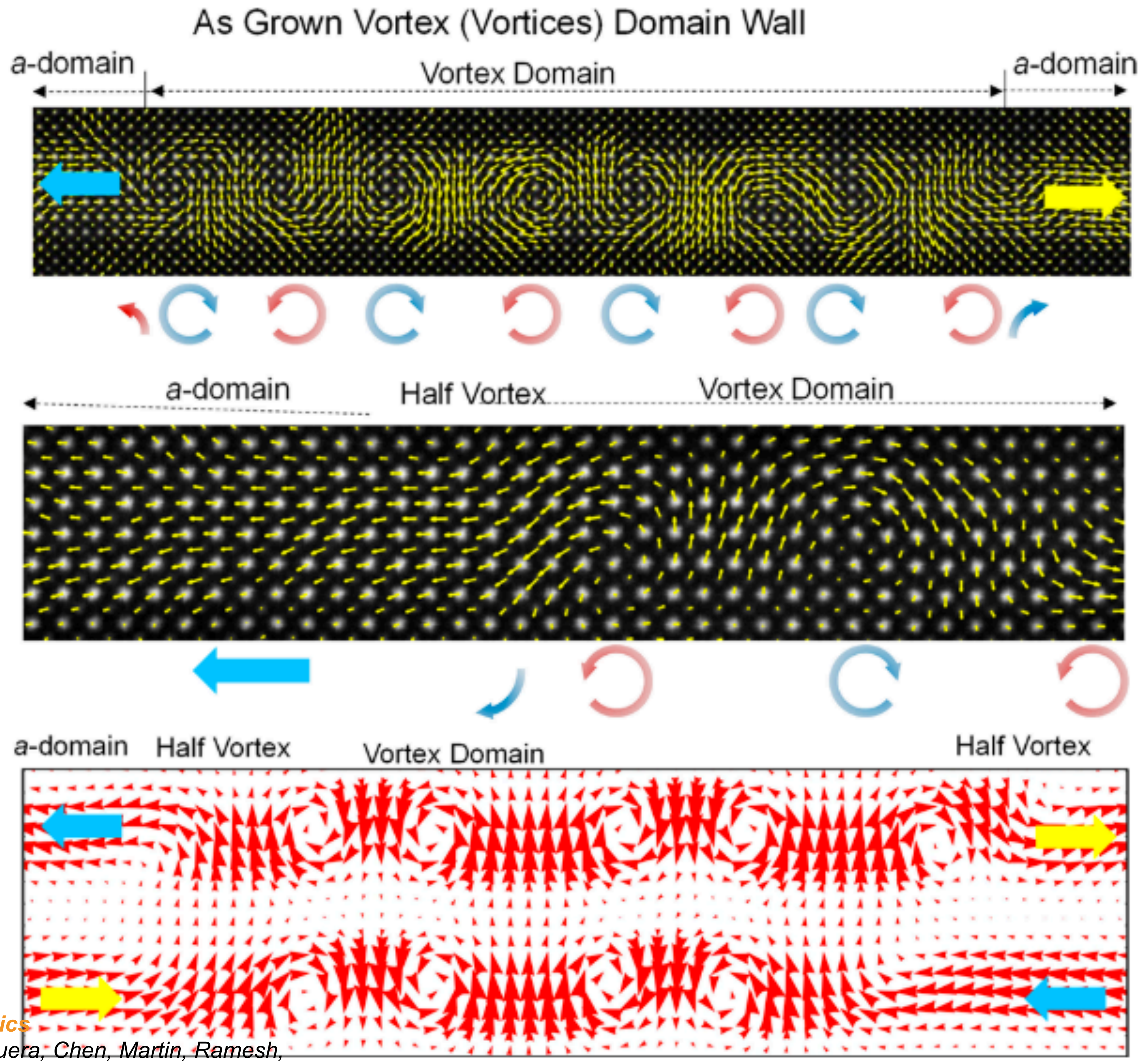

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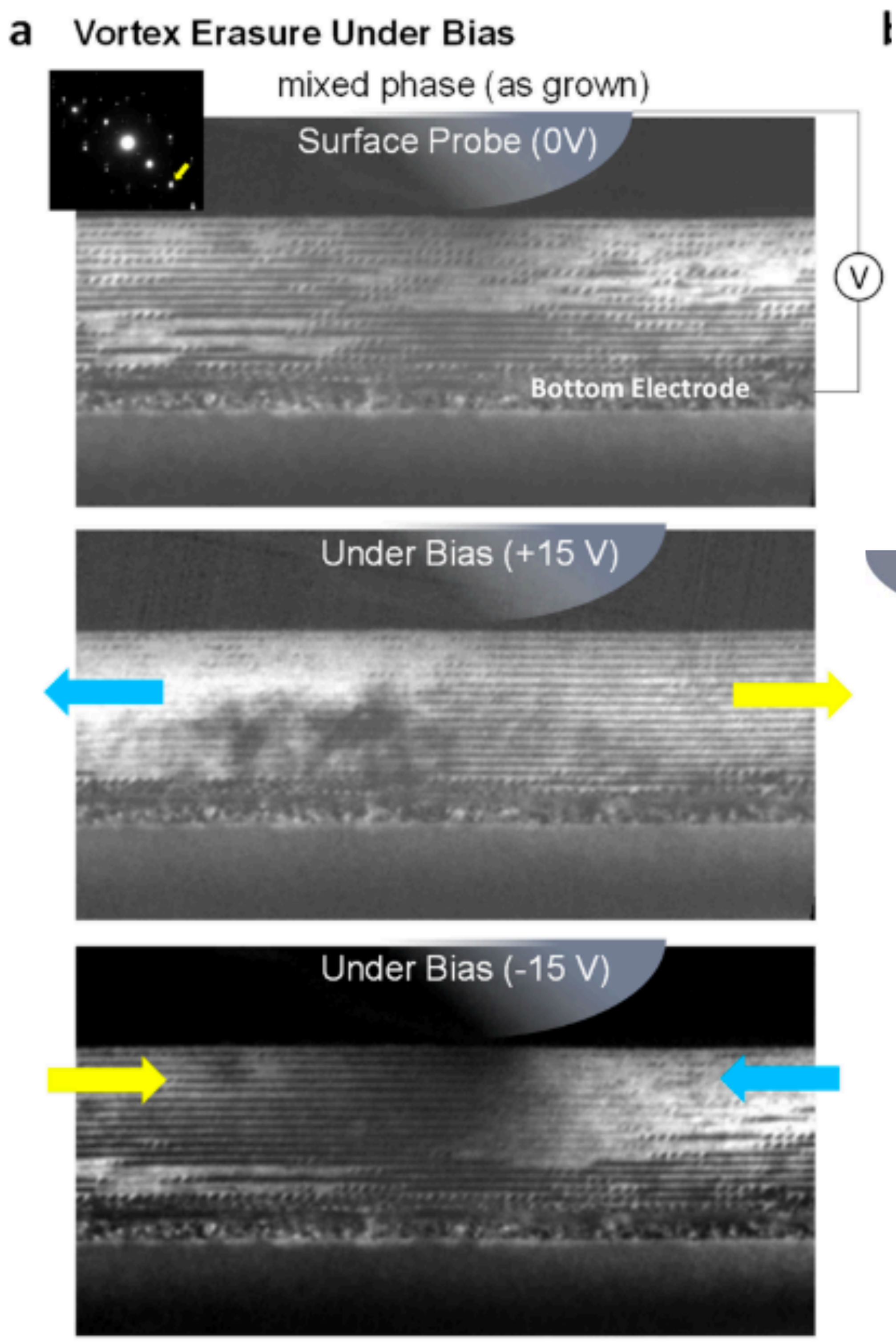

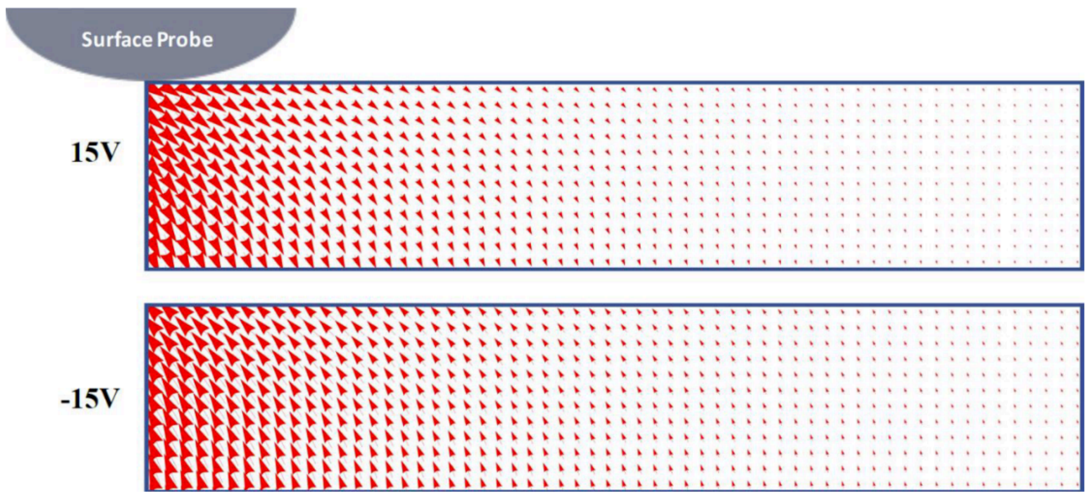

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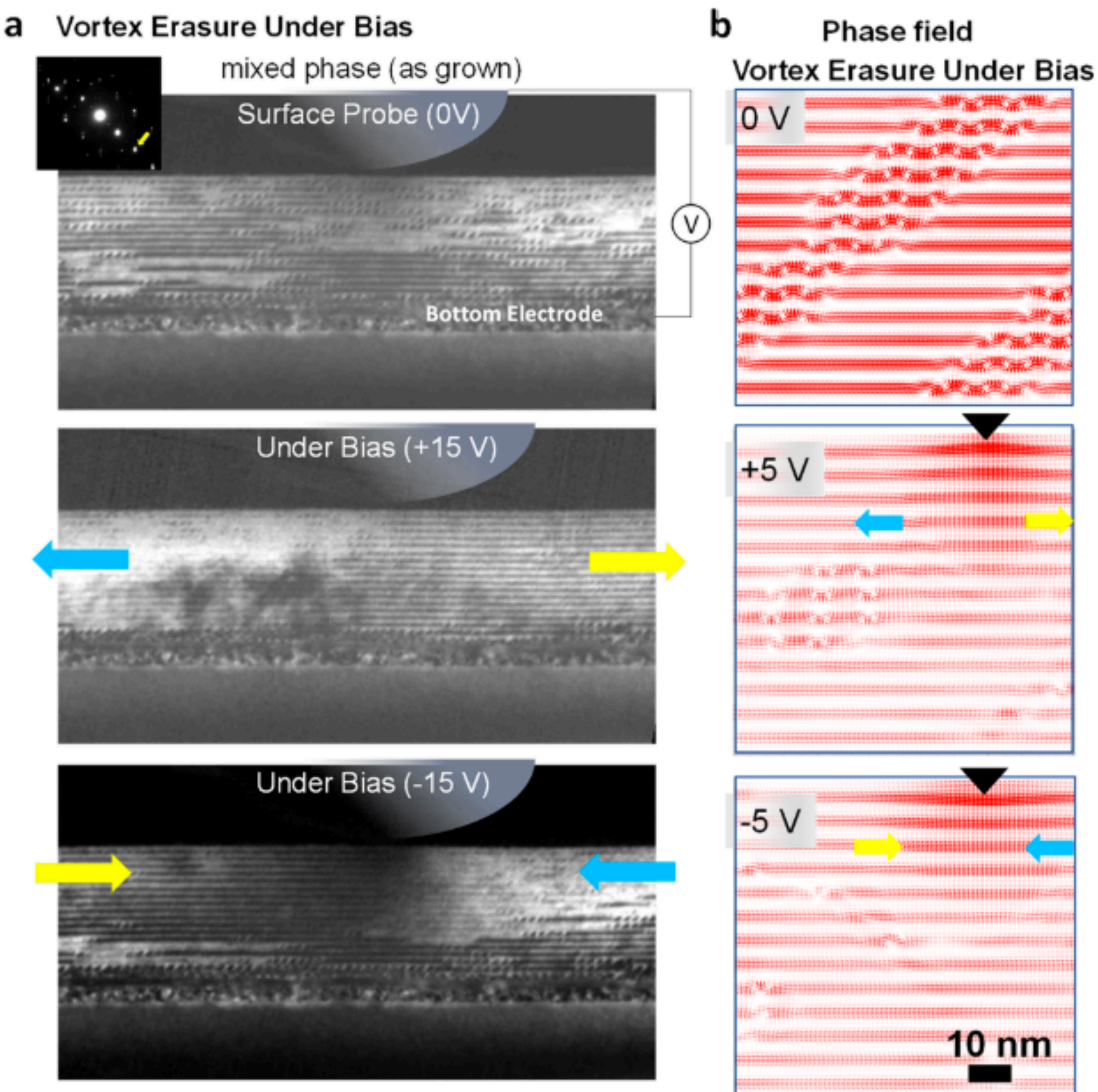

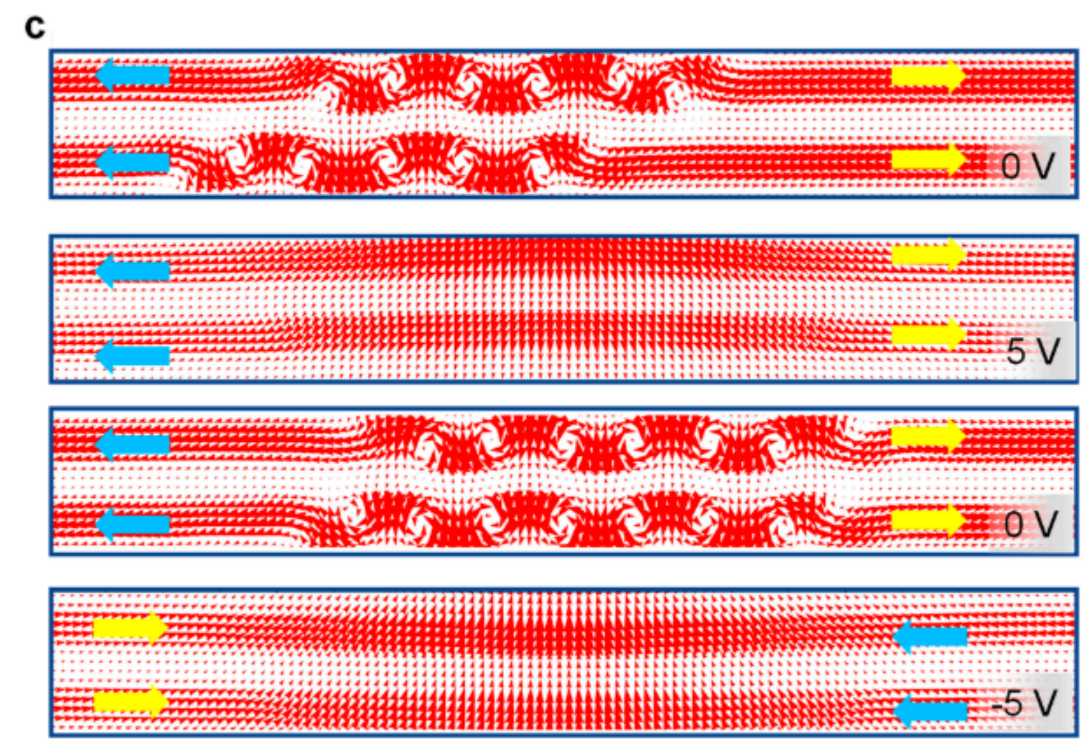

⇛ reversible switching between the in-plane polarised charged domain wall and the vortex domain wall

Vortex Domain Walls in Ferroelectrics
Hong, Das, Nelson, Yadav, Wu, Junquera, Chen, Martin, Ramesh, Nano Letters 21 3533 (2021)

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Thank you!

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